Efficient Linear Algebra methods for Data Mining
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## Team members involved in this work - Support

## Past:

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## Support:

- National Science Foundation


## Introduction, background, and motivation

Common goal of data mining methods: to extract meaningful information or patterns from data. Very broad area - includes: data analysis, machine learning, pattern recognition, information retrieval, ...
> Main tools used: linear algebra; graph theory; approximation theory; optimization; ...
> In this talk: emphasis on dimension reduction techniques and the interrelations between techniques
$>$ Focus on two main problems

- Information retrieval
- Face recognition
$>$ and 3 types of dimension reduction methods
- Standard subspace methods [SVD, Lanczos]
- Graph-based methods
- multilevel methods


## The problem

$>$ Given $d \ll m$ find a mapping $\Phi: x \in \mathbb{R}^{m} \longrightarrow y \in \mathbb{R}^{d}$
> Mapping may be explicit (e.g., $\left.y=V^{T} x\right)$
> Or implicit (nonlinear)


## Practically:

Given $\boldsymbol{X} \in \mathbb{R}^{m \times n}$, we want to find a low-dimensional representation $\boldsymbol{Y} \in \mathbb{R}^{d \times n}$ of $\boldsymbol{X}$
> Two classes of methods: (1) projection techniques and (2) nonlinear implicit methods.

## Example 1: The 'Swill-Roll' (2000 points in 3-D)

Original Data in 3-D


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## 2-D ‘reductions':




Eigenmaps


ONPP


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## Example 2: Digit images (a sample of 30)



## 2-D 'reductions':



## Projection-based Dimensionality Reduction

Given: a data set $X=\left[x_{1}, x_{2}, \ldots, x_{n}\right]$, and $d$ the dimension of the desired reduced space $\boldsymbol{Y}$.
Want: a linear transformation from $X$ to $\boldsymbol{Y}$


$$
\begin{aligned}
& \boldsymbol{X} \in \mathbb{R}^{m \times n} \\
& V \in \mathbb{R}^{m \times d} \\
& \boldsymbol{Y}=\boldsymbol{V}^{\top} \boldsymbol{X} \\
& \rightarrow \quad \boldsymbol{Y} \in \mathbb{R}^{d \times n}
\end{aligned}
$$

$>m$-dimens. objects $\left(x_{i}\right)$ 'flattened' to $d$-dimens. space $\left(y_{i}\right)$
Constraint: The $y_{i}$ 's must satisfy certain properties
> Optimization problem

## Linear Dimensionality Reduction: PCA

> In PCA projected data must have maximum variance, i.e., we need to maximize over all orthogonal $m \times d$ matrices $V$ :

$$
\sum_{i}\left\|\boldsymbol{y}_{i}-\frac{1}{n} \sum_{j} \boldsymbol{y}_{j}\right\|_{2}^{2}=\cdots=\operatorname{Tr}\left[\boldsymbol{V}^{\top} \overline{\boldsymbol{X}} \overline{\boldsymbol{X}}^{\top} \boldsymbol{V}\right]
$$

Where: $\bar{X}=X\left(I-\frac{1}{n} 11^{T}\right)==$ origin-recentered version of $X$
$>$ Solution $V=\{$ dominant eigenvectors $\}$ of the covariance matrix == Set of left singular vectors of $\bar{X}$
$>$ Solution $V$ also minimizes 'reconstruction error' ..

$$
\sum_{i}\left\|x_{i}-V V^{T} x_{i}\right\|^{2}=\sum_{i}\left\|x_{i}-V y_{i}\right\|^{2}
$$

$>.$. and it also maximizes [Korel and Carmel 04] $\sum_{i, j}\left\|\boldsymbol{y}_{i}-\boldsymbol{y}_{j}\right\|^{2}$

## Information Retrieval: Vector Space Model

Given: 1) set of documents (columns of a matrix $A$ ); 2) a query vector q. Entry $a_{i j}$ of $A=$ frequency of term $i$ in document $j+$ weighting.

> Queries ('pseudo-documents') $q$ represented similarly to columns
Problem: find columns of $A$ that best match $q$

## Vector Space Model and the Truncated SVD

$>$ Similarity metric: angle between column $\boldsymbol{A}_{j,:}$ and query $q$

## Use Cosines:

$$
\frac{\left|\boldsymbol{q}^{T} \boldsymbol{A}_{:, j}\right|}{\left\|\boldsymbol{A}_{:, j}\right\|_{2}\|\boldsymbol{q}\|_{2}}
$$

$>$ To rank all documents compute the similarity vector:

$$
s=\boldsymbol{A}^{T} \boldsymbol{q}
$$

> Not very effective. Problems : polysemy, synonymy, ...
$>$ LSI: replace matrix $\boldsymbol{A}$ by low rank approximation

$$
A=U \Sigma V^{T} \quad \rightarrow \quad A_{k}=U_{k} \Sigma_{k} V_{k}^{T} \quad \rightarrow \quad s_{k}=A_{k}^{T} q
$$

$>U_{k}$ : term space, $V_{k}$ : document space.
$>$ Called TSVD - Expensive, hard to update, ..

## New similarity vector:

$$
s_{k}=A_{k}^{T} \boldsymbol{q}=V_{k} \Sigma_{k} U_{k}^{T}
$$

$>$ How to select $k$ ?
Issues: $>$ Computational cost (memory + computation)
$>$ Problem with updates
$>$ Alternative: SDD; Less memory but cost still an issue.
$>$ Alternative: polynomial approximation. $s_{k} \approx \phi_{k}\left(A^{T} A\right) A^{T} q$ where $\phi_{k}=$ deg. $k$ polynom.
> Yet another alternative: use Lanczos vectors instead of singular vectors [Ruhe and Blom, 2005]

## IR: Use of the Lanczos algorithm

* Joint work with Jie Chen
> Lanczos is good at catching large (and small) eigenvalues: can compute singular vectors with Lanczos, \& use them in LSI
> Can do better: Use the Lanczos vectors directly for the projection..
> First advocated by: K. Blom and A. Ruhe [SIMAX, vol. 26, 2005]. Use Lanczos bidiagonalization.
$>$ Use a similar approach - But directly with $\boldsymbol{A} \boldsymbol{A}^{T}$ or $\boldsymbol{A}^{T} \boldsymbol{A}$.


## IR: Use of the Lanczos algorithm (1)

$>$ Let $\boldsymbol{A} \in \mathbb{R}^{m \times n}$. Apply the Lanczos procedure to $M=\boldsymbol{A} \boldsymbol{A}^{T}$. Result:

$$
Q_{k}^{T} A A^{T} Q_{k}=T_{k}
$$

with $Q_{k}$ orthogonal, $T_{k}$ tridiagonal.
$>$ Define $s_{i} \equiv$ orth. projection of $A b$ on subspace span $\left\{Q_{i}\right\}$

$$
s_{i}:=Q_{i} Q_{i}^{T} A b
$$

$>s_{i}$ can be easily updated from $s_{i-1}$ :

$$
s_{i}=s_{i-1}+q_{i} \boldsymbol{q}_{i}^{T} A b
$$

## IR: Use of the Lanczos algorithm (2)

$>$ If $n<m$ it may be more economial to apply Lanczos to $M=$ $\boldsymbol{A}^{T} \boldsymbol{A}$ which is $n \times n$. Result:

$$
\bar{Q}_{k}^{T} A^{T} A \bar{Q}_{k}=\bar{T}_{k}
$$

> Define:

$$
t_{i}:=A \bar{Q}_{i} \bar{Q}_{i}^{T} b
$$

$>$ Project $b$ first before applying $\boldsymbol{A}$ to result.

## Why does this work?

$>$ First, recall a result on Lanczos algorithm [YS 83]
Let $\left\{\lambda_{j}, u_{j}\right\}=j$-th eigen-pair of $M$ (label $\downarrow$ )

$$
\frac{\left\|\left(I-Q_{k} Q_{k}^{T}\right) u_{j}\right\|}{\left\|Q_{k} Q_{k}^{T} u_{j}\right\|} \leq \frac{K_{j}}{T_{k-j}\left(\gamma_{j}\right)} \frac{\left\|\left(I-Q_{1} Q_{1}^{T}\right) u_{j}\right\|}{\left\|Q_{1} Q_{1}^{T} u_{j}\right\|}
$$

where

$$
\gamma_{j}=1+2 \frac{\lambda_{j}-\lambda_{j+1}}{\lambda_{j+1}-\lambda_{n}}, \quad K_{j}=\left\{\begin{array}{ll}
1 & j=1 \\
\prod_{i=1}^{j-1} \frac{\lambda_{i}-\lambda_{n}}{\lambda_{i}-\lambda_{j}} & j \neq 1
\end{array},\right.
$$

and $T_{l}(x)=$ Chebyshev polynomial of 1 st kind of degree $l$.
This has the form

$$
\left\|\left(I-Q_{k} Q_{k}^{T}\right) u_{j}\right\| \leq c_{j} / T_{k-j}\left(\gamma_{j}\right)
$$

where $\boldsymbol{c}_{j}=$ constant independent of $k$
$>$ Result: Distance between unit eigenvector $u_{j}$ and Krylov subspace $\operatorname{span}\left(Q_{k}\right)$ decays fast (for small $j$ )
$>$ Consider component of difference between $A b-s_{k}$ along left singular directions of $\boldsymbol{A}$. If $\boldsymbol{A}=\boldsymbol{U} \Sigma \boldsymbol{V}^{T}$, then $\boldsymbol{u}_{j}$ 's (columns of $\boldsymbol{U}$ ) are eigenvectors of $M=\boldsymbol{A} \boldsymbol{A}^{T}$. So:

$$
\begin{aligned}
\left|\left\langle A b-s_{k}, u_{j}\right\rangle\right| & =\left|\left\langle\left(I-Q_{k} Q_{k}^{T}\right) A b, u_{j}\right\rangle\right| \\
& =\left|\left\langle\left(I-Q_{k} Q_{k}^{T}\right) u_{j}, A b\right\rangle\right| \\
& \leq\left\|\left(I-Q_{k} Q_{k}^{T}\right) u_{j}\right\|\|A b\| \\
& \leq c_{j}\|A b\| T_{k-j}^{-1}\left(\gamma_{j}\right)
\end{aligned}
$$

$>\left\{s_{i}\right\}$ converges rapidly to $\boldsymbol{A b}$ in directions of the major left singular vectors of $\boldsymbol{A}$.
$>$ Similar result for left projection sequence $t_{j}$
$>$ Here is a typical distribution of eigenvalues of $M$ : [Matrix of size $1398 \times 1398$ ]

> Convergence toward first few singular vectors very fast -

Advantages of Lanczos over polynomial filters:
(1) No need for eigenvalue estimates
(2) Mat-vecs performed only in preprocessing

Disadvantages:
(1) Need to store Lanczos vectors;
(2) Preprocessing must be redone when $\boldsymbol{A}$ changes.
(3) Need for reorthogonalization - expensive for large $k$.

## Tests: IR

Information
retrieval
datasets

|  | \# Terms | \# Docs | \# queries | sparsity |
| :--- | ---: | ---: | ---: | ---: |
| MED | 7,014 | 1,033 | 30 | 0.735 |
| CRAN | 3,763 | 1,398 | 225 | 1.412 |

Med dataset.

## Cran dataset.




Kalamata, 09-05-2008

## Average query times

## Med dataset

## Cran dataset.



## Average retrieval precision

## Med dataset



Cran dataset


Retrieval precision comparisons

## In summary:

> Results comparable to those of SVD ...
> .. at a much lower cost. [However not for the same dimension $k$ ]

## Thanks:

> Helpful tools and datasets widely available. We used TMG [developed at the U. of Patras (D. Zeimpekis, E. Gallopoulos)]

## Problem 2: Face Recognition - background

Problem: We are given a database of images: [arrays of pixel values]. And a test (new) image.


Question: Does this new image correspond to one of those in the database?

## Difficulty

$>$ Different positions, expressions, lighting, ..., situations :


Common approach: eigenfaces - Principal Component Analysis technique

Example: Occlusion. See recent paper by John Wright et al.

Right: 50\% pixels randomly changed


## Eigenfaces

- Consider each picture as a one-dimensional colum of all pixels
- Put together into an array $A$ of size \#_pixels $\times \#$ _images .

- Do an SVD of $\boldsymbol{A}$ and perform comparison with any test image in low-dim. space
- Similar to LSI in spirit - but data is not sparse.

Idea: replace SVD by Lanczos vectors (same as for IR)

## Tests: Face Recognition

Tests with 2 well-known data sets:
ORL 40 subjects, 10 sample images each - example:

\# of pixels: $112 \times 92$ TOT. \# images : 400
AR set 126 subjects - 4 facial expressions selected for each [natural, smiling, angry, screaming] - example:

\# of pixels: $112 \times 92$ \# TOT. \# images: 504

## Tests: Face Recognition

Recognition accuracy of Lanczos approximation vs SVD

ORL dataset


AR dataset


Vertical axis shows average error rate. Horizontal = Subspace dimension

## GRAPH-BASED TECHNIQUES

## Laplacean Eigenmaps (Belkin-Niyogi-02)

$>$ Not a linear (projection) method but a Nonlinear method
$>$ Starts with k-nearest-neighors graph
> Defines the graph Laplacean $L=D-$ $W$. Simplest:
$D=\operatorname{diag}(\operatorname{deg}(i)) ; \quad w_{i j}= \begin{cases}1 & \text { if } j \in N_{i} \\ 0 & \text { else }\end{cases}$
with $N_{i}=$ neighborhood of $i(\operatorname{excl} . i) ; \operatorname{deg}(i)=\left|N_{i}\right|$

## A few properties of graph Laplacean matrices

$>$ Let $L=$ any matrix s.t. $L=D-W$, with $D=\operatorname{diag}\left(d_{i}\right)$ and

$$
w_{i j} \geq 0, \quad d_{i}=\sum_{j \neq i} w_{i j}
$$

Property 1: for any $x \in \mathbb{R}^{n}$ :

$$
x^{\top} \boldsymbol{L} x=\frac{1}{2} \sum_{i, j} w_{i j}\left|x_{i}-x_{j}\right|^{2}
$$

Property 2: (generalization) for any $\boldsymbol{Y} \in \mathbb{R}^{d \times n}$ :

$$
\operatorname{Tr}\left[Y L Y^{\top}\right]=\frac{1}{2} \sum_{i, j} w_{i j}\left\|y_{i}-y_{j}\right\|^{2}
$$

Property 3: For the particular $L=I-\frac{1}{n} \mathbf{1 1}^{\top}$

$$
\boldsymbol{X} \boldsymbol{L} \boldsymbol{X}^{\top}=\overline{\boldsymbol{X}} \overline{\boldsymbol{X}}^{\top}==n \times \text { Covariance matrix }
$$

[Proof: 1) $L$ is a projector: $L^{\top} L=L^{2}=L$, and 2) $\boldsymbol{X} L=\overline{\boldsymbol{X}}$ ]
$>$ Consequence-1: PCA equivalent to maximizing $\sum_{i j}\left\|y_{i}-y_{j}\right\|^{2}$
$>$ Consequence-2: what about replacing trivial $L$ with something else? [viewpoint in Koren-Carmel'04]

Property 4: (Graph partitioning) If $x$ is a vector of signs $( \pm 1)$ then

$$
x^{\top} \boldsymbol{L} x=4 \times(\text { 'number of edge cuts') }
$$

edge-cut $=$ pair $(i, j)$ with $x_{i} \neq x_{j}$
> Consequence: Can be used for partitioning graphs, or 'clustering' [take $p=\operatorname{sign}\left(u_{2}\right)$, where $u_{2}=2$ nd smallest eigenvector..]

## Return to Laplacean eigenmaps approach

Laplacean Eigenmaps *minimizes*

$$
\mathcal{F}_{E M}(\boldsymbol{Y})=\sum_{i, j=1}^{n} w_{i j}\left\|y_{i}-y_{j}\right\|^{2} \quad \text { subject to } \quad Y D Y^{\top}=I
$$

## Notes:

1. Motivation: if $\left\|x_{i}-x_{j}\right\|$ is small (orig. data), we want $\left\|y_{i}-y_{j}\right\|$ to be also small (low-D data)
2. Note Min instead of Max as in PCA [counter-intuitive]
3. Above problem uses original data indirectly through its graph
$>$ Problem translates to:

$$
\left\{\begin{array}{c}
\min _{\boldsymbol{Y} \in \mathbb{R}^{d \times n}} \operatorname{Tr}\left[\boldsymbol{Y}(\boldsymbol{D}-\boldsymbol{W}) \boldsymbol{Y}^{\top}\right] . \\
\boldsymbol{Y} \boldsymbol{D} \boldsymbol{Y}^{\top}=\boldsymbol{I}
\end{array}\right.
$$

$>$ Solution (sort eigenvalues increasingly):

$$
(D-W) u_{i}=\lambda_{i} D u_{i} ; \quad y_{i}=u_{i}^{\top} ; \quad i=1, \cdots, d
$$

$>$ Note: an $n \times n$ sparse eigenvalue problem [In 'sample' space]
$>$ Note: can assume $D=I$. Amounts to rescaling data. Problem becomes

$$
(I-W) u_{i}=\lambda_{i} u_{i} ; \quad y_{i}=u_{i}^{\top} ; \quad i=1, \cdots, d
$$

Intuition:
Graph Laplacean and 'unit' Laplacean are very different: one involves a sparse graph (More like a discr. differential operator). The other involves a dense graph. (More like a discr. integral operator).
They should be treated as the inverses of each other.
> Viewpoint confirmed by what we learn from Kernel approach

## Locally Linear Embedding (Roweis-Saul-00)

> LLE is very similar to Eigenmaps. Main differences:

1) Graph Laplacean matrix is replaced by an 'affinity' graph
2) Objective function is changed: want to preserve graph
1. Graph: Each $x_{i}$ is written as a convex combination of its $k$ nearest neighbors:
$x_{i} \approx \Sigma w_{i j} x_{j}, \quad \sum_{j \in N_{i}} w_{i j}=1$
$>$ Optimal weights computed ('local calculation') by minimizing


$$
\left\|x_{i}-\Sigma w_{i j} x_{j}\right\| \quad \text { for } \quad i=1, \cdots, n
$$

## 2. Mapping:

The $y_{i}$ 's should obey the same 'affinity' as $x_{i}$ 's $\rightsquigarrow$
Minimize:

$$
\sum_{i}\left\|y_{i}-\sum_{j} w_{i j} y_{j}\right\|^{2} \quad \text { subject to: } \quad Y \mathbf{1}=0, \quad Y Y^{\top}=I
$$

Solution:

$$
\left(I-W^{\top}\right)(I-W) u_{i}=\lambda_{i} u_{i} ; \quad y_{i}=u_{i}^{\top}
$$

$>\left(I-W^{\top}\right)(I-W)$ replaces the graph Laplacean of eigenmaps

## Locally Preserving Projections (He-Niyogi-03)

- LPP is a linear dimensionality reduction technique
> Recall the setting:
Want $\boldsymbol{V} \in \mathbb{R}^{m \times d} ; \boldsymbol{Y}=\boldsymbol{V}^{\top} \boldsymbol{X}$

$>$ Starts with the same neighborhood graph as Eigenmaps: $L \equiv$ $D-W=$ graph 'Laplacean'; with $D \equiv \operatorname{diag}\left(\left\{\Sigma_{i} w_{i j}\right\}\right)$.
$>$ Optimization problem is to solve

$$
\min _{Y \in \mathbb{R}^{d \times n}, Y D Y^{\top}=I} \Sigma_{i, j} w_{i j}\left\|y_{i}-y_{j}\right\|^{2}, \quad Y=V^{\top} X .
$$

$>$ Difference with eigenmaps: $\boldsymbol{Y}$ is a projection of $\boldsymbol{X}$ data
$>$ Solution (sort eigenvalues increasingly)

$$
\boldsymbol{X} L \boldsymbol{X}^{\top} \boldsymbol{v}_{i}=\lambda_{i} \boldsymbol{X} \boldsymbol{D} \boldsymbol{X}^{\top} \boldsymbol{v}_{i} \quad \boldsymbol{y}_{i,:}=\boldsymbol{v}_{i}^{\top} \boldsymbol{X}
$$

$>$ Note: essentially same method in [Koren-Carmel'04] called 'weighted PCA' [viewed from the angle of improving PCA]

## ONPP (Kokiopoulou and YS '05)

> Orthogonal Neighborhood Preserving Projections
> Can be viewed as a linear version of LLE
> Uses the same graph as LLE. Objective: preserve the affinity graph (as in LEE) *but* by means of an orthogonal projection
$>$ Objective function

$$
\Phi(\boldsymbol{Y})=\Sigma_{i}\left\|y_{i}-\Sigma_{j} w_{i j} y_{j}\right\|^{2} \quad \text { Constraint: } \boldsymbol{Y}=V^{\top} \boldsymbol{X}, V^{\top} \boldsymbol{V}=\boldsymbol{I}
$$

$>$ Notice that

$$
\Phi(\boldsymbol{Y})=\left\|\boldsymbol{Y}-\boldsymbol{Y} W^{\top}\right\|_{F}^{2}=\cdots=\operatorname{Tr}\left[V^{\top} \boldsymbol{X}\left(\boldsymbol{I}-\boldsymbol{W}^{\top}\right)(I-W) \boldsymbol{X}^{\top} V\right]
$$

## Resulting problem:

$$
\min _{\substack{\mathcal{\mathbb { P } ^ { m \times d _ { j } }} \\ V^{\top} V=I}} \operatorname{Tr}[V^{\top} \underbrace{X\left(I-W^{\top}\right)(I-W) X^{\top}}_{M} V]
$$

Solution: Columns of $V=$ eigenvectors of $M$ associated with smallest $d$ eigenvalues
$>$ Can be computed as $d$ lowest left singular vectors of

$$
\boldsymbol{X}\left(I-W^{\top}\right)
$$

## A unified view

| Method | Object. (min) | Constraint |
| :--- | :---: | :---: |
| PCA/MDS | $\operatorname{Tr}\left[\boldsymbol{V}^{\top} \boldsymbol{X}\left(-\boldsymbol{I}+e e^{\top}\right) \boldsymbol{X}^{\top} \boldsymbol{V}\right]$ | $\boldsymbol{V}^{\top} \boldsymbol{V}=\boldsymbol{I}$ |
| LLE | $\operatorname{Tr}\left[\boldsymbol{Y}\left(\boldsymbol{I}-W^{\top}\right)(\boldsymbol{I}-W) \boldsymbol{Y}^{\top}\right]$ | $\boldsymbol{Y} \boldsymbol{Y}^{\top}=\boldsymbol{I}$ |
| Eigenmaps | $\operatorname{Tr}\left[\boldsymbol{Y}(\boldsymbol{I}-W) \boldsymbol{V}^{\top}\right]$ | $\boldsymbol{Y} \boldsymbol{Y}^{\top}=\boldsymbol{I}$ |
| LPP | $\operatorname{Tr}\left[\boldsymbol{V}^{\top} \boldsymbol{X}(\boldsymbol{I}-W) \boldsymbol{X}^{\top} \boldsymbol{V}\right]$ | $\boldsymbol{V}^{\top} \boldsymbol{X} \boldsymbol{X}^{\top} \boldsymbol{V}=\boldsymbol{I}$ |
| ONPP | $\operatorname{Tr}\left[\boldsymbol{V}^{\top} \boldsymbol{X}\left(\boldsymbol{I}-W^{\top}\right)(\boldsymbol{I}-W) \boldsymbol{X}^{\top} \boldsymbol{V}\right]$ | $\boldsymbol{V}^{\top} \boldsymbol{V}=\boldsymbol{I}$ |
| LDA | $\operatorname{Tr}\left[\boldsymbol{V}^{\top} \boldsymbol{X}(\boldsymbol{I}-\boldsymbol{H}) \boldsymbol{X}^{\top} \boldsymbol{V}\right]$ | $\boldsymbol{V}^{\top} \boldsymbol{X} \boldsymbol{X}^{\top} \boldsymbol{V}=\boldsymbol{I}$ |

$>$ Let $M=I-W=$ a Laplacean matrix $\left(-I+e e^{\top}\right.$ for PCA/MDS); or the LLE matrix $(\boldsymbol{I}-W)\left(I-W^{\top}\right)$, or geodesic distance matrix (ISOMAP).
> All techniques lead to one of two types of problems

$$
\operatorname{Tr}\left[\boldsymbol{Y} M Y^{\top}\right]
$$

$>$ First type is:

$$
\begin{aligned}
& \min ^{\prime} \in \mathbb{R}^{d \times n} \\
& \boldsymbol{Y}^{\top}=I
\end{aligned}
$$

> $\boldsymbol{Y}$ obtained from solving an eigenvalue problem
$>$ LLE, Eigenmaps (normalized), ..

$>G$ is either the identity matrix or $\boldsymbol{X D} \boldsymbol{X}^{\top}$ or $\boldsymbol{X} \boldsymbol{X}^{\top}$.
$>$ Low-Dim. data: $\boldsymbol{Y}=\boldsymbol{V}^{\top} \boldsymbol{X}$
Important observation: 2nd is just a projected version of the 1st, i.e., approximate eigenvectors are sought in Span $\{\boldsymbol{X}\}$ [RayleighRitz procedure]
$>$ Problem is of dim. $m$ (dim. of data) not $n$ (\# of samples).
> This difference can be mitigated by resorting to Kernels..

## Graph-based methods in a supervised setting

> Subjects of training set are known (labeled). Q: given a test image (say) find its label.




Question: Find label (best match) for test image.

Methods can be adapted to supervised mode by building the graph to take into account class labels. Idea is simple: Build $G$ so that nodes in the same class are neighbors. If $c=\#$ classes, $G$ will consist of $c$ cliques.
> Matrix $W$ will be block-diagonal

$$
W=\operatorname{diag}\left(W_{1}, W_{2}, \cdots, W_{c}\right)
$$

$>$ Easy to see that $\operatorname{rank}(W)=n-c$.
$>$ Can be used for LPP, ONPP, etc..

TIME FOR A MATLAB DEMO

## Supervised learning experiments: digit recognition

$>$ Set of 390 images of digits (39 of each digit)


$>$ Each picture has $20 \times 16=320$ pixels.

$>$ Select any one of the digits
 and try to recognize it among the 389 remaining images

> Methods: KNN, PCA, LPP, ONPP

## One word about KNN-classifiers

$>$ Simple idea of 'vote' - get $k$ nearest neighbors.
$>$ Assigned label = 'most common label among these neibhbors'


## MULTILEVEL METHODS

## Multilevel techniques

> Divide and conquer paradigms as well as multilevel methods in the sense of 'domain decomposition'
> Main principle: very costly to do an SVD [or Lanczos] on the whole set. Why not find a smaller set on which to do the analysis without too much loss?
$>$ Tools used: graph coarsening, divide and conquer -

## Multilevel techniques: Hypergraphs to the rescue

General idea: Given $\boldsymbol{X}=\left[x_{1}, \cdots, x_{n}\right] \in \mathbb{R}^{m \times n}$ find another set ('coarsened set') $\hat{X}=\left[\hat{x}_{1}, \cdots, \hat{x}_{k}\right] \in \mathbb{R}^{m \times k}$
$>\hat{X}$ should be a good representative of $\boldsymbol{X}-$
$>$ then find projector from $\mathbb{R}^{m}$ to $\mathbb{R}^{d}$ based on this subset
$>$ Main tool used: graph coarsening.
$>$ We will describe hypergraph-based techniques

## Hypergraphs

A hypergraph $\boldsymbol{H}=(\boldsymbol{V}, \boldsymbol{E})$ is a generalizaition of a graph
> $V=$ set of vertices $V$
$\boldsymbol{\nabla} \boldsymbol{E}=$ set of hyperedges. Each $e \in \boldsymbol{E}$ is a nonempty subset of $V$
$>$ Standard undirected graphs: each e consists of two vertices.
$>$ degree of $e=|e|$
$>$ degree of a vertex $v=$ number of hyperedges $e$ s.t. $x \in e$.
$>$ Two vertices are neighbors if there is a hyperedge connecting them

> Canonical hypergraph representation for sparse data (e.g. text)

## Hypergraph Coarsening

> Coarsening a hypergraph $\boldsymbol{H}=(\boldsymbol{V}, \boldsymbol{E})$ means finding a 'coarse' approximation $\hat{H}=(\hat{\boldsymbol{V}}, \hat{\boldsymbol{E}})$ to $\boldsymbol{H}$ with $|\hat{\boldsymbol{V}}|<|\boldsymbol{V}|$, which tries to retain as much as possible of the structure of the original hypergraph
> Idea: repeat coarsening recursively.
> Result: succession of smaller hypergraphs which approximate the original graph.
> Several methods exist. We use 'matching', which successively merges pairs of vertices
> Used in most graph partitioning methods: hMETIS, Patoh, zoltan,
> Algorithm successively selects pairs of vertices to merge - based on measure of similarity of the vertices.

## Application: Multilevel Dimension Reduction

## Main Idea:

to a certain level. Then use the resulting data set $\hat{X}$ to find projector from $\mathbb{R}^{m}$ to $\mathbb{R}^{d}$. This projector can be used to project the original data or any new data.

> Main gain: Dimension reduction is done with a much smaller set. Hope: not much loss compared to using whole data

## Application to text mining

> Recall common approach:

1. Scale data [e.g. TF-IDF scaling: ]
2. Perform a (partial) SVD on resulting matrix $X \approx \boldsymbol{U}_{d} \Sigma_{d} V_{d}^{T}$
3. Process query by same scaling (e.g. TF-IDF)
4. Compute similarities in $d$-dimensional space: $s_{i}=\left\langle\hat{q}, \hat{x}_{i}\right\rangle /\|\hat{q}\|\left\|\hat{x}_{i}\right\|$ where $\left[\hat{x}_{1}, \hat{x}_{2}, \ldots, \hat{x}_{n}\right]=V_{d}^{T} \in \mathbb{R}^{d \times n} ; \quad \hat{q}=\Sigma_{d}^{-1} U_{d}^{T} \bar{q} \in \mathbb{R}^{d}$
> Multilevel approach: replace SVD (or any other dim. reduction) by dimension reduction on coarse set. Only difference: TF-IDF done on the coarse set not original set.

## Tests

Three public data sets used for experiments: Medline, Cran and NPL (cs.cornell.edu)
$>$ Coarsening to a max. of 4 levels.

| Data set | Medline | Cran | NPL |
| :--- | ---: | ---: | ---: |
| \# documents | 1033 | 1398 | 11429 |
| \# terms | 7014 | 3763 | 7491 |
| sparsity (\%) | $0.74 \%$ | $1.41 \%$ | $0.27 \%$ |
| \# queries | 30 | 225 | 93 |
| avg. \# rel./query | 23.2 | 8.2 | 22.4 |

## Results with NPL

## Statistics

| Level | coarsen. <br> time | \# <br> doc. | optimal |  |
| :---: | :---: | :---: | :---: | :---: |
|  | optimal avg. |  |  |  |
| precision |  |  |  |  |

## Precision-Recall curves



CPU times for preprocessing (Dim. reduction part)


## Conclusion

> So how is this related to intitial title of "efficient algorithms in data mining"?
> Answer: All these eigenvalue problems are not cheap to solve..
> .. and cost issue does not seem to bother practitioners too much for now..
$>$ Ingredients that will become mandatory:
1 Avoid the SVD
2 Fast algorithms that do not sacrifice quality.
3 In particullar: Multilevel approaches
4 Multilinear algebra [tensors]

